Additions and Corrections

Demonstration by ^{13}C NMR Spectroscopy of Regiospecific Carbon−Carbon Coupling during Fischer−Tropsch Probe Reactions [*J. Am. Chem. Soc.* **1999**, *121*, 6497−6498]. Brian E. Mann, Michael L. Turner, Ruhksana Quyoum, Nyoman Marsih, and Peter M. Maitlis*

Page 6497, caption to Figure 1, line 2: $^{13}CO/H_2$ should read $^{12}CO/H_2$.

Page 6498, caption to Figure 2, line 2: $^{13}CO/H_2$ should read $^{12}CO/H_2$.

Page 6498, caption to Figure 3, line 2: $^{13}CH_3{}^{13}CH{=}^{13}CH_2$ should read $^{13}CH_3{}^{13}CH{=}^{12}CH_2$; $^{13}CH_3{}^{13}CH_2{}^{13}CH{=}^{13}CH_2$ should read $^{13}CH_3{}^{13}CH_2{}^{12}CH{=}^{12}CH_2$; line 3: $^{13}CH_3{}^{13}CH_2(^{13}CH_2)_n{}^{13}CH{=}^{13}CH_2$ should read $^{13}CH_3{}^{13}CH_2(^{12}CH_2)_n{}^{12}CH{=}^{12}CH_2$; line 4: $^{13}CH_2$ (from ^{13}CO) should read $^{12}CH_2$ (from ^{12}CO).

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Book Reviews

Advances in Quantitative Structure Property Relationships. Volume 2. Edited by Marvin Charton (Pratt Institute) and Barbara I. Charton (St. John's University). JAI Press Inc.: Stamford, CT. 1999. xi + 257 pp. $109.50. ISBN 0-7623-0067-1.

As chemists we have the enormous advantage of dealing with specific compounds which are characterized by a unique structural formula. Once a structural formula of a compound is written out, all the properties of the compound are already defined: physical, chemical, biological, and technological. If only we could read the code, then we could know everything about that compound just from its structural formula. While great strides have been made in predicting properties by the ever more powerful molecular orbital methods, we are still a very long way from being able to understand from molecular orbital procedures how chemical structure drives most properties.

The alternative is to use a QSPR/QSAR method. In principle, this means obtaining a database of the structures and the property of interest in numerical form and attempting to find a relationship between various "descriptors" of the molecules and the magnitude of the property in question. In this respect, descriptors can be any quantitatively defined function which can either be obtained from the structural formula alone or be measured. The area of QSAR which deals with biological activities has made tremendous advances over the last 25 years. No pharmaceutical company can now operate without a department of computational chemistry, which is concerned with QSAR and drug mechanism and activity.

By contrast, QSPR, particularly as concerns the correlation of physical and technological properties with structure, has been much slower in its application by the chemical and allied industries. Much fundamental work has been carried out over the last 50 years, and indeed, in principle QSPR is more straightforward than QSAR. However, until recently a lot of the work was concerned with the fundamental theory, and much of it dealt with data sets which related to compounds of the same general type, above all with hydrocarbons. However, the picture is now changing rapidly, and industry in particular is becoming aware of the enormous advantages of QSPR techniques in helping to define strategies for synthesis. Clearly, if one can have some kind of a prediction for the likely changes in properties of interest depending of the structure of the compound, this can be of enormous help in speeding up a synthetic search for more effective compounds. The present series of advances attempts to bring together QSPR results from various areas of chemical research. These endeavors are very much to be welcomed. The present volume consists of four chapters from diverse areas.

In the first chapter, Phillip S. Magee from Biosar explores the energetics of binding in chromatography and other absorption phenomena. Topics discussed include binding energies and retention times for chromatography on clay, silica, alumina, cellulose, and paper. The binding of organic compounds to soils is also included. This chapter illustrates the wide range of applicability and emphasizes that QSPR not only is useful for predictions but at least as importantly can give information about the fundamental mechanism of such interactions.

The second chapter, by G. Churchani, M. Mishima, R. Notario, and J. L. Abboud, is a joint effort between Spain, Venezuela, and Japan, dealing with structural effects on gas-phase reactivities. It mainly concerns extensions of the Hammet equation (and its later modifications, especially those of Taft and Yukawa-Tsuno) to the gas phase. The material treated is divided into reactions involving ionic reagents and those involving only neutral agents and products. Both topics are covered authoritatively.

John Deardon of Moore University, Liverpool, UK, covers the prediction of melting points, one of the most difficult to achieve by QSPR because it involves crystal forces and crystal structures, and many compounds crystallize in more than one form with different melting points. Because of this, most attempts to predict melting point have been carried out on subsets with limited functional diversity, although attempts are now being made to find equations that relate to diverse data sets.

The final chapter in the volume, by Marvin Charton of the Pratt Institute of New York, describes applications of the intermolecular force model to peptide and protein QSAR. Attempts to deal with bioactivity in terms of the distinct steps of transport, receptor interaction, and chemical reaction are described.

The four chapters of the present volume provide a diverse set of QSPR applications. The book is well written and produced and should be of value to researchers in a multitude of fields.

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